Optimization in Chemical Engineering
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Lecture – 54
Applications of Optimization
(Contd.)

Welcome to lecture 54. In this week 11, we are talking about various Applications of Optimization. In today's lecture, we will talk about 2 different applications; the first application is taken from chemical reaction engineering and we will talk about a CSTR problem. In the next example we will talk about a Transportation Problem. So, let us start with first problem.

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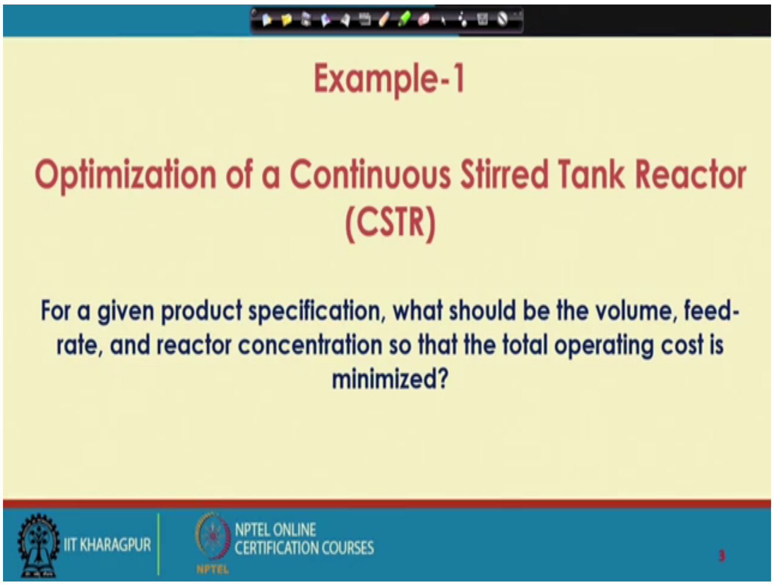

So, for the CSTR problem, the problem is as follows. For a given product specification, what should be the volume feed rate and the reactor concentration so that the total operating cost is minimized? So, you are going to solve an optimization problem related to continuous stirred tank reactor. So, there is a reaction taking place for a given product specification, what should be the volume feed rate and the reactor concentration so that the total operating cost is minimized? Of course, we will be given some components of the operating cost.

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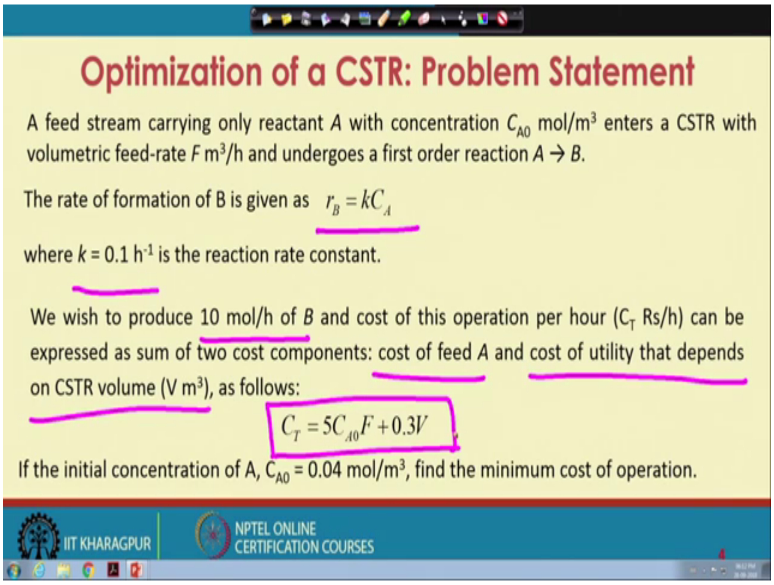

So, let us now define the problem in more details. A feed stream carrying only reactant A with concentration C A 0 mole per meter cube enters a CSTR with volumetric feed rate F meter cube per hour and undergoes the first order reaction such as A to B. The rate of formation of B is given as r B equal to k into C A, where r B is the rate of formation of B; k is the reaction rate constant and the value of the reaction rate constant k is given as 0.1 hour inverse and C A is the concentration of A in the reactor in the unit of mole per meter cube. We want to produce 10 moles per hour of B.

So, this is the product specification. We want to produce 10 mole per hour of B and the cost of this operation per hour can be expressed as a sum of 2 cost components cost of feed A and cost of utility that depends on the CSTR volume. And, the expression is the total operating cost in say rupees per hour is 5 into C A 0 into F plus 0.3 into V.

So, the first part 5 in to C A 0 into F is the component corresponding to cost of feed rate and the next part corresponds to the cost of utility and it depends on the CSTR volume. So, the cost depends on the feed rate the volume of the reactor and of course, the initial concentration of A in the feed stream. Note that C A 0 into F is basically moles of A that is entering per hour. So, with the initial concentration of A is given as C A 0 equal to 0.4 mole per meter cube, we have to find the minimum cost of operation.

So, how do we solve this problem? So, the problem is that you have a CSTR; where a simple first order reaction such as A to B takes place the reaction rate constraint is given this 0.1 hour inverse. We want to produce 10 moles per hour of B. So, the total operating cost is the cost of feed plus utility cost that depends on volume. So, if we fix the initial concentration of A in the feed stream as 0.04 moles per meter cube; what will be the minimum cost of operation?

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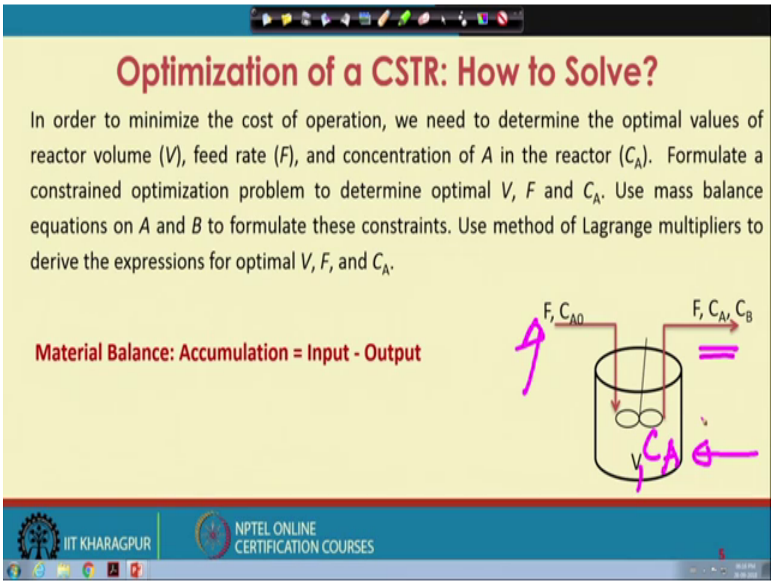

So, in order to minimize the cost of operation, we need to determine the optimal values of reactor volume V, the feed rate F and the concentration of A in the reactor that is C A which is this. Note that this is CSTR so; the concentration of A in the reactor is same as the concentration of A in the exit stream. Formulate a constrained optimization problem to determine optimal values of V. There is volume of reactor F, the feed rate and C A the concentration of A in the reactor or in the exit stream.

So, to define or formulate the constrained optimization problem, we have to use mass balance equations on A and B to formulate these constraints. See if we apply mass balance equations on A and B will be able to formulate this constraint. Note that in the CSTR episteme containing only A with the specified concentration comes in, a reaction takes place and the exit steam has the same flow rate as the inlet steam.

So, the volume remains constant. So, you can write down the mass balance equation on A and mass balance equation on B; we have a constrained on the product specification. So, considering this, we will have 2 mass balance equations which will correspond to the 2 constraints. Then, we will write down or formulate the objective function and these 2 constraints will lead to a constrained optimization problem which can be solved using say Lagrange Multipliers method. So, let us see how we formulate the problem first.

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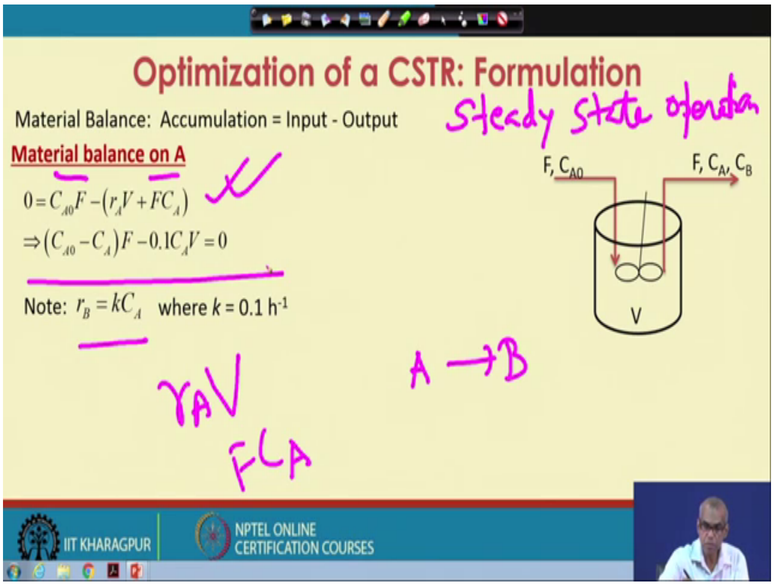

Mass balance is nothing but a statement such as accumulation equal to input minus output. So, the mass balance on A will be accumulation of A which is 0 because it is a CSTR; we consider steady state operation. So, accumulation is 0 so, then input. Input is the amount of A that is coming into the reactor. So, that is C A 0 into F minus output. So, there are 2 terms; one is A goes to B.

So, that causes depletion in A and also A goes out with the exit steam. So, the depletion of A due to reaction will be r A into V. Note that r A will be same as r B which will be equal to k into C A and the amount of A that goes out with the exits steam is flow rate into concentration; so, F into C A. So, you are able to write this first equation which can be rearranged to this. So, this gives me the mass balance equation on A; similarly you can write the mass balance equation on B.

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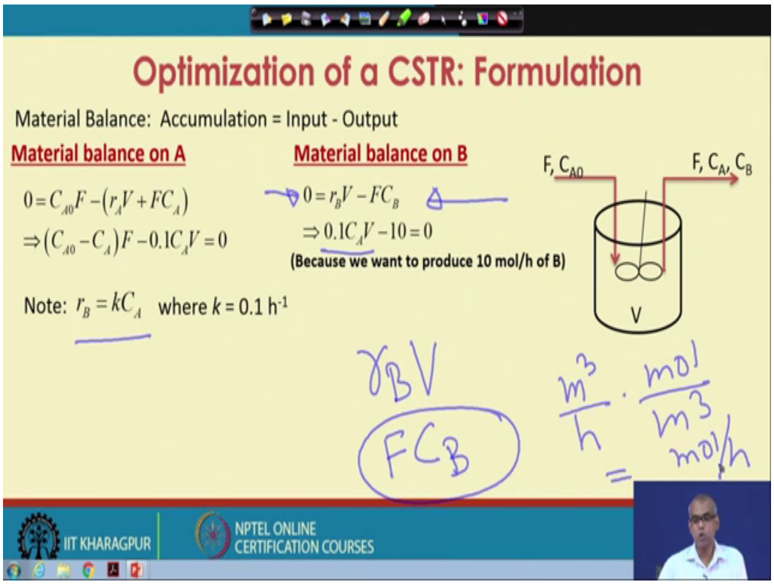

Again, the accumulation of B is 0; then, input of B is same as formation of B. So, that is r B V because B is being form from A due to the reaction A to B and then, B goes out with the exits stream. So, that will be F the volumetric flow rate into the concentration. So, r B V minus F C B is the mass balance equation for component B. So, for r B let us put k into C A or 0.1 into C A. So, I get this term and F C B is the amount of B that is going out with the exit stream. Let us look at the unit.

So, F is volumetric flow rate. So, meter cube per hour and concentration is mole per meter cube. So, F C B is mole per hour. So, F into C B moles per hour is basically will set it to 10 because we want to produce 10 moles per hour of B. So, that is why FCB is being set as 10 to meet the product specification. So, this leads to this equation for mass balance on B. So, we now have 2 mass balance equations on A and B respectively. So, these are 2 constraints.

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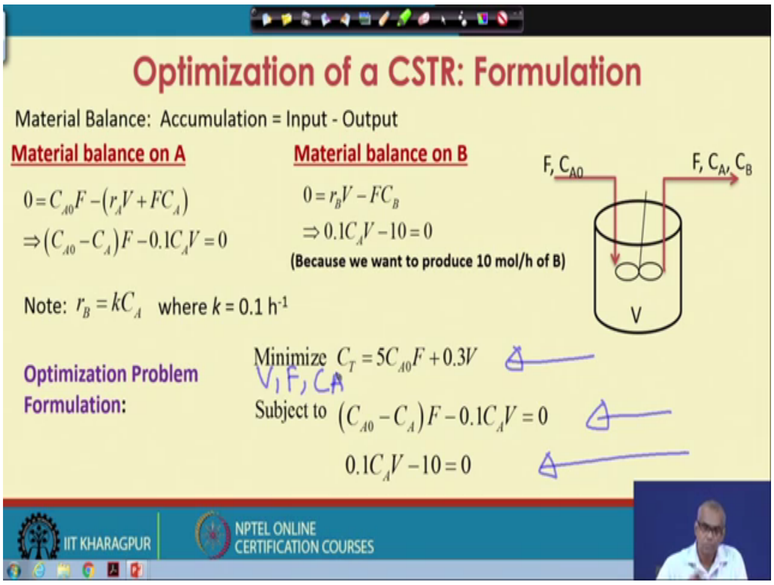

So, let us now formulate the optimization problem formally. First the objective function, we want to minimize the total hourly cost of operation which is given as 5 C A 0 into F plus 0.3 V subject to the mass balance equation on A mass balance equation on B and what are the decision variables? The decision variables are V, F and C A. So, this is the optimization problem that you have to solve. So, basically you have an optimization problem with 2 equality constraints.

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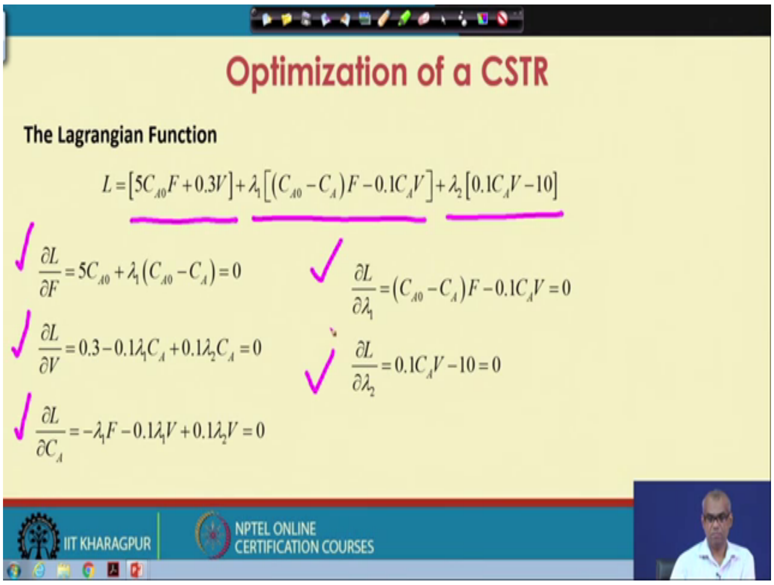

So, I can formulate the Lagrangian function. The objective function, then Lagrangian multiplier into the first constraint and then another Lagrangian multiplier into the second constraint; so, we have the Lagrangian function. So, let us now apply the first order necessary condition for optimality which is the derivative of the Lagrangian with respect to all the state variables and the Lagrange multipliers will be equal to 0.

So, del L del F will be equal to 0; del L del V will be equal to 0; del L del C A will be equal to 0 and also del L del lambda 1 equal to 0 del L del lambda equal to lambda 2 equal to 0. So, then I get 5 equations. These conditions gives me a set of 5 equation which needs to be solved simultaneously to find out volume flow rate concentration and of course, you will also get lambda 1 and lambda 2.

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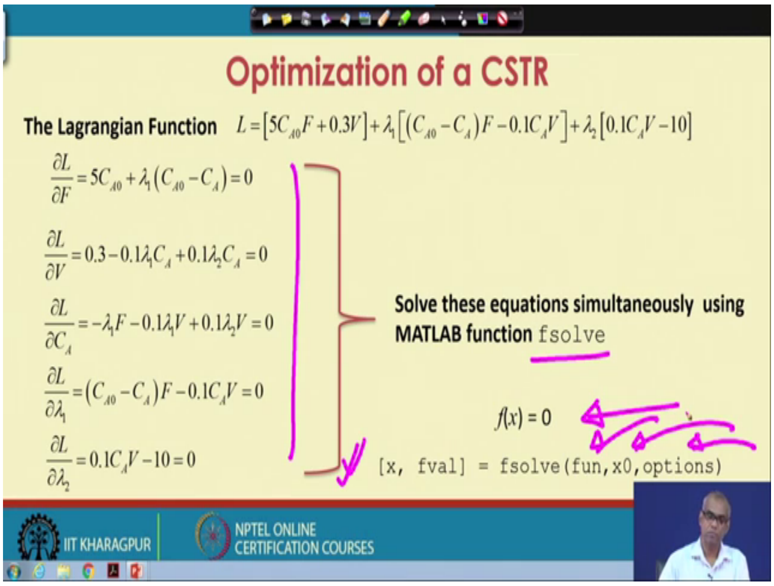

So, we have now 5 equations. These are simultaneous equations which we can solve using the MATLAB function f solve; you know that f solve solves an equation such as f x equal to 0 f x equal to 0 represents a set of simultaneous equations which may be non-linear equations and you are now familiar with the syntax for f solve. You have to define a function, where you will write down all this simultaneous equations. You will supply the initial guess and you can also supply options as a argument to give specific instructions to the solver f solve.

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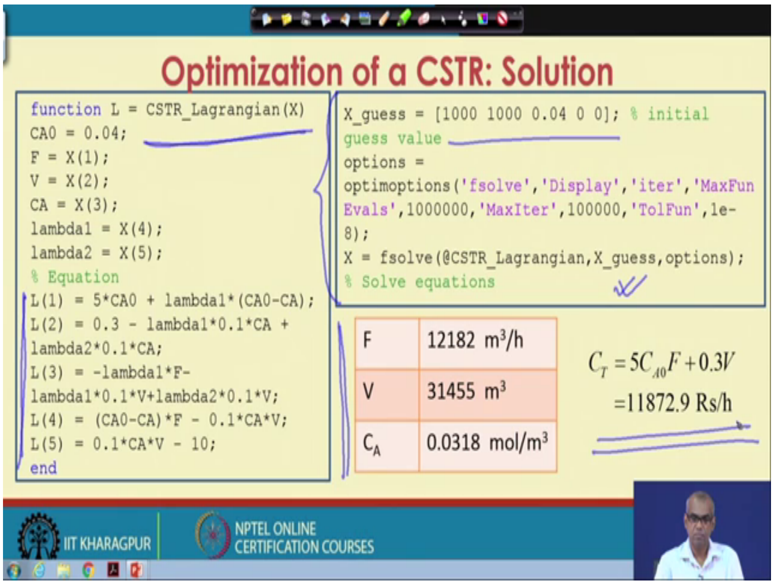

So, this is the MATLAB code that you can use, to define a function known as CSTR Lagrangian which defines all the equations that needs to be solved simultaneously and then, we give a guess value initial guess value, we define options and then call f solve. So, you define a function give the name CSTR underscore Lagrangian or whatever name you want. So, you create an m file. So, the file will have extension dot m and then, these statements either you can enter on the script file or enter on the command mode.

If you write a file, you give some name to it save it as dot m file and then, run the file. If you run you will get these are solutions for flow rate volume and the concentration of A. So, this will correspond to the minimum hourly cost of operation which for this case is 11872.9 rupees per hour. So, this is how you can solve the given optimization problem related to hourly cost minimization of a CSTR when a target product specification is given.

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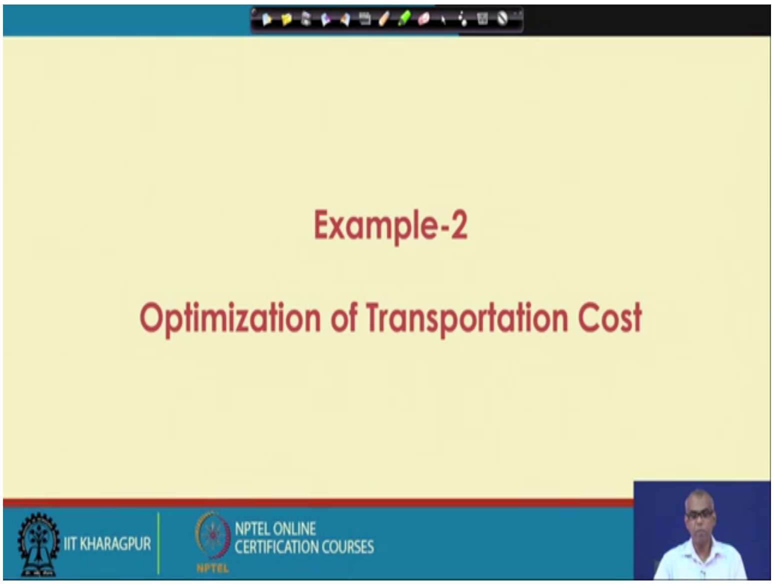

So, next problem, we take is Optimization of Transportation Cost.

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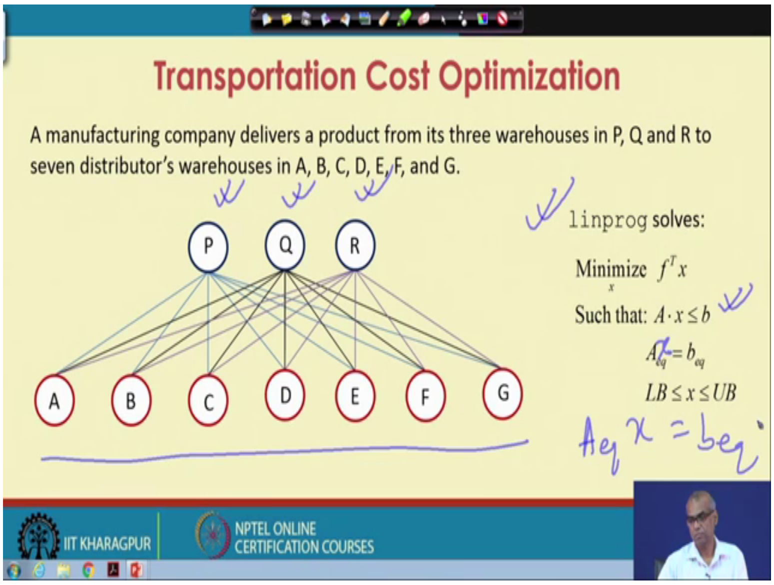

Consider a manufacturing company it produces a product and it has 3 warehouses in P Q and R and then, there are 7 distributors. So, there are 7 distributors' warehouses in A B C D E F G. So, the manufacturing company delivers a product from its 3 warehouses in P Q R to 7 distributors warehouses in A B C D E F G, we have to minimize the total cost of operation. Of course, the cost of transportation from P Q R to each of these 7 distributors will be given.

We have already discussed that such problems will lead to a linear programming problems and MATLABs linprog can be used to solve such problem. So, MATLABs linprog solves an objective function f transpose x; where, f transpose where f vector contains the cost coefficients and the constraints are A x less or equal to b which are linear in equality type constrained and e equality x equal to b equality which is linear equality type constraints and then lower bounds on the decision variables.

So, if you can cast your problem in this form you can solve using the solver linprog and given linear programming problem you will be able to solve you will be able to cast in the format specifiers.

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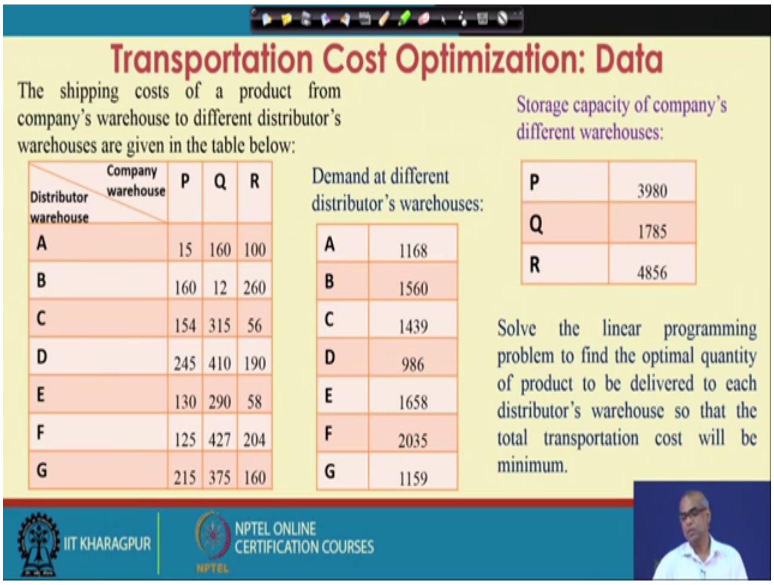

So, now let us look at the data associated with the transportation problem. The shipping costs of a product from company's warehouse to different distributor's warehouses are given in the table you now see on the screen.

So, we have to read as the cost of shipping from P to A is 15. So, this is the unit of cost; in any unit of cost that is a rupees or dollar unit of cost. So, that is 15. P to B it is 160 and so on and so forth. Similarly Q to A is 160 Q to D is 410 and so on and so forth. Similarly from R to A will be 100. R to G will be 160 and so on and so forth.

So, the total data of shipping of a product from company's warehouse to different distributor's warehouse are given. The next the demand at all the 7 distributor's warehouses are given. So, there are 7 distributors' warehouses and each warehouse has a demand associated with it and these are given. Then, the companies 3 different warehouses have different capacity for storage. So, they are also specified. So, companies three warehouses storage capacity as specified; 7 distributor warehouses demands are given and cost of the product from company warehouse to each of the distributors warehouses are given.

So, we have to solve the linear programming problem to find the optimal quantity of product to be delivered to each distributor's warehouse so that the total transportation cost will be minimum. So, we have to formulate a linear programming problem and solve the problem to find out what is the optimal quantity of product to be delivered to each distributors warehouse from companies warehouses so that the total transportation cost is minimum. So, this is a standard linear programming problem.

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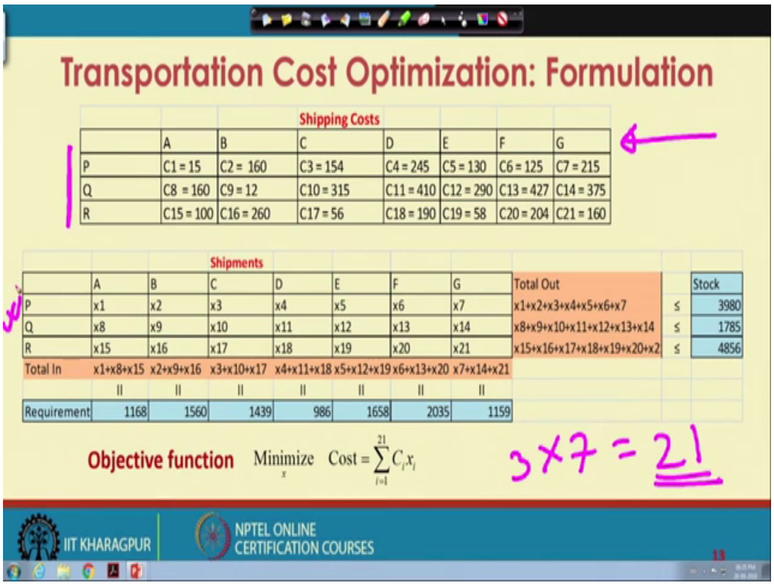

So, the shipping cost are again shown in the table. So, P Q R are the company warehouses and these are the distributors warehouses. So, the variables for the problem are the quantity of the product that needs to be shipped from 3 company warehouses to 7 distributors warehouses. So, we have 3 into 7 equal to 21 decision variables.

So, those are x 1, x 2 up to x 21. So, now, let us look at this table. So, this table allows us to define the constraints, we have 2 types of constraints; one is the storage and the other is the demands. So, let us say the demands are exactly to be satisfied. So, we can write like x 1 plus x 8 plus x 15. So, this corresponds to x 1 quantity received from company warehouse P; x 8 quantity received from company warehouse Q and x 15 quantity received from company warehouse R.

So, the distributor warehouse in A receives x 1 plus x 2 plus x 15. So, this should be greater or equal to the demand at distributors A. Let us say we are first, we are first saying that the demands will be exactly met. So, the quantity that is received in A will be equal to the demand at A.

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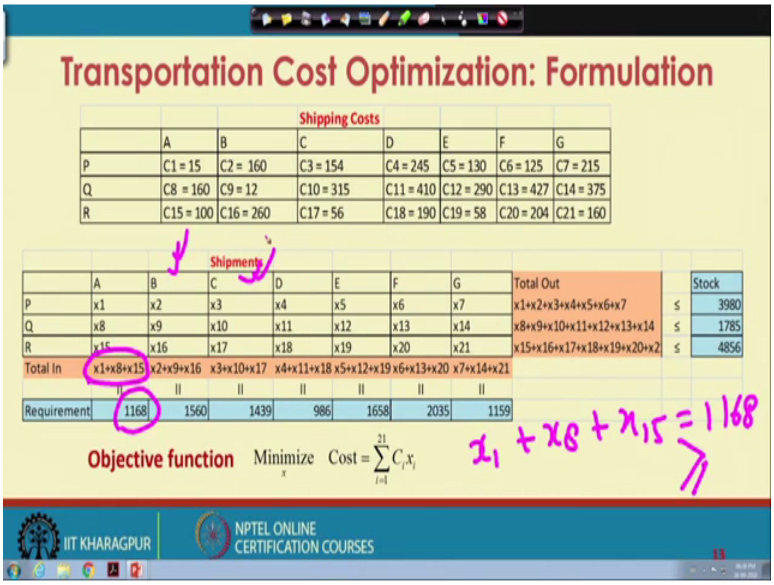

So, we will write x 1 plus x 8 plus 15 is equal to 1168. So, x 1 plus x 8 plus x 15 is equal to 1168. Note that you can also write greater or equal to 1168. Similarly, you can write down the constraints for all the 7 warehouses. So, this is for demand. Now, each company warehouse are limited or fixed storage specified storage capacity. So, x 1, x 2, x 3, x 4, x 5, x 6 and x 7; these goes out from company's warehouse P to 7 distributor's warehouses. So, some of these x 1, x 2, x 3, x 4, x 5, x 6 and x 7 must be less or equal to the storage capacity of company warehouse A.

So, that is why we write this first constraint. Similarly, we write second constraint as well as third constraint. So, we have a linear programming problem, where these storage capacity constraints are satisfied as less or equal to and the demand constraints are being satisfied as equal to. The demand constraints can also be formulated as greater or equal to and you will get the same solution.

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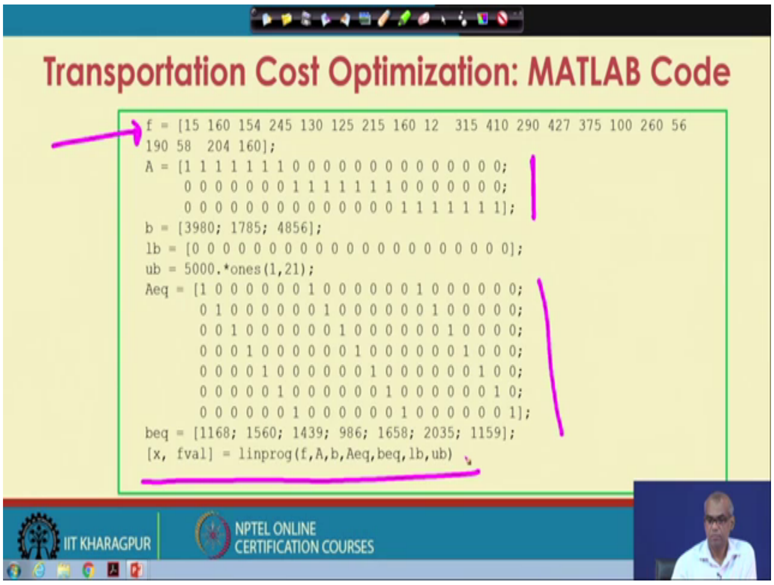

So, now you can use the linprog solver of MATLAB. So, the cost coefficients as shown in the table are written as a f vector then this is the matrix for the inequality constraints; this is for the equality constraints and then you call the linprog solver.

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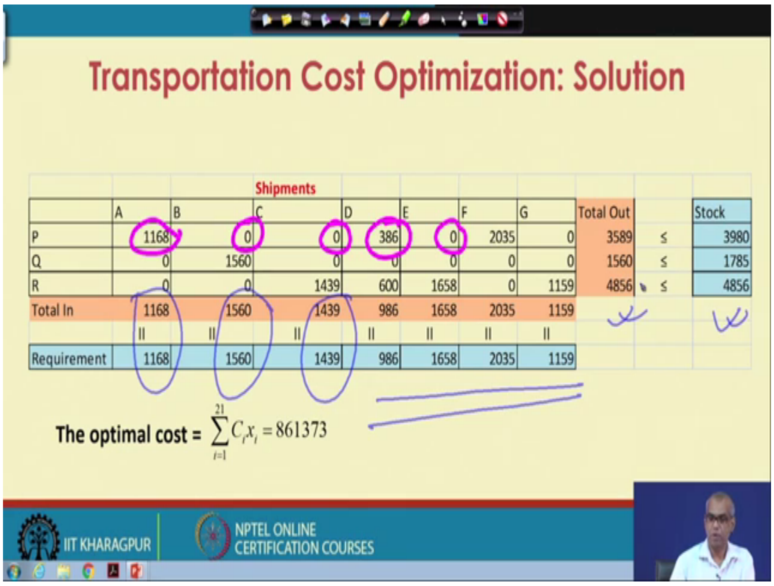

So, the solution you obtain is as follows. So, these are the solutions all 21. Note that the equality constraints, the demand is specified as equality constraints are exactly satisfied. Similarly, the storage capacity constraints are also satisfied.

So, this is how we can solve a transportation problem by formulating as a linear programming problem and using the linprog solver of MATLAB.

With this we conclude lecture 54 here.